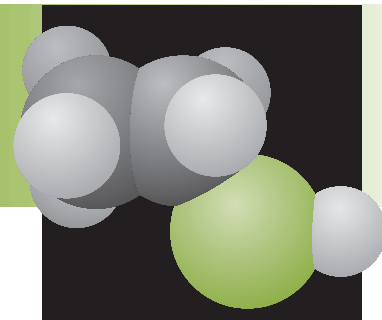


CHEMICALS

Project Fact Sheet



BIOCATALYSIS UNDER EXTREME CONDITIONS FOR THE CHEMICAL INDUSTRY

BENEFITS

- Energy savings of nearly 70 trillion Btu in 2020
- Produces higher yields with less waste
- Increases process efficiency

APPLICATIONS

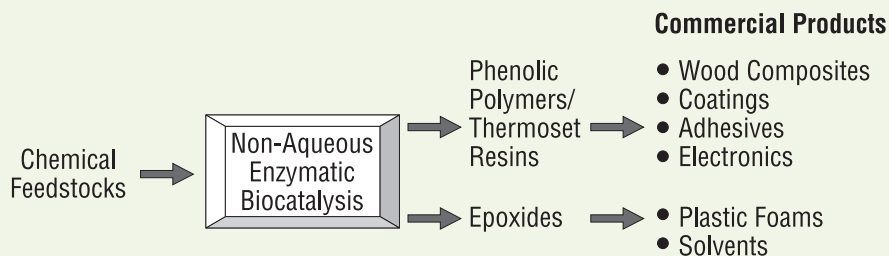
Industry support has been gained for this effort from a number of companies with an interest in alternative chemical processing, which will help hasten the marketing of biocatalysts. The availability of enzymes for use in organic solvents will benefit all sectors of the chemical industry, as well as the pharmaceutical, agrochemical, and food industries. The petrochemical industry will also apply the new processes to its smaller-volume oxidative chemical reactions. Phenolic polymerization and alkene epoxidation are a significant portion of the industry's production cycle and the development of better techniques will have an impact on the industry.

ENZYMATIC TRANSFORMATIONS WILL BE APPLIED TO CRITICAL CHEMICAL PROCESSES

Biocatalysts (i.e., enzymes) can be used to initiate major chemical reactions, such as the direct polymerization of phenols or the direct oxidation of propylene. Manufacturers who require polyphenols or propylene oxide (PO) in their production processes may reduce their costs substantially by deriving them biocatalytically. This project focuses on developing the core pre-competitive technology needed for conducting these enzymatic reactions in nonaqueous media.

Phenolic polymers have an annual market value of more than \$3 billion and are required to manufacture thermoset resins, which are used in wood composites, abrasives, coatings and adhesives, electronics, and other products. Currently, the Novolac process is used for producing polyphenols, and requires formaldehyde, which is a toxic and carcinogenic chemical that is difficult to recover. Replacing the Novolac process with enzymatic polymerization would eliminate formaldehyde from the process and increase the stability of the resin materials. Likewise, the present chlorhydrin process used for PO production requires alkaline conditions, creates undesirable byproducts, and produces wastes that must be treated.

CHEMICAL INTERMEDIATES THROUGH ENZYMES



Enzymatic catalysis can be used to produce polymers that are used in the manufacture of many consumer products.



Project Description

Goal: To develop active and stable biocatalysts as commercially relevant alternatives to chemical processing, using oxidases to carry out phenolic polymerization and to epoxidize directly propylene and other alkenes.

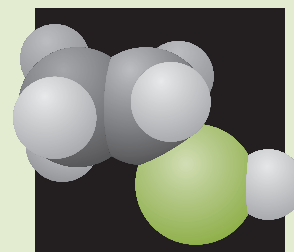
Four issues will be addressed by this precompetitive research: (1) The activity and stability of oxidative enzymes must be improved, (2) the structural features that promote high enzyme activity and stability in organic solvents must be elucidated and a fundamental understanding of enzyme reactions in organic media obtained, (3) processes using activated/stabilized oxidases for phenolic polymerization and alkene epoxidation must be developed, and (4) the progress of the work must be assessed along with an preliminary economic and environmental analysis of the impact of the technology. Additionally, the general techniques for this technology must be simple and scalable so it is commercially viable.

Strategies of the research will include engineering the enzyme using small effector molecules, employing ligands to enhance enzyme solubility in organic media, and cross-linking and immobilizing enzyme molecules for long-term stabilization in dehydrated environments. Fundamental and applied investigations of potential industrial applications will be pursued to determine their commercial value.

Peroxidase catalysis uses an oxidative biotransformation to generate phenolic polymers without using formaldehyde; successful bench tests make this closer to commercialization. Alkene epoxidation (e.g., the preparation of propylene oxide) is a higher-risk venture, but it is of great interest to several industrial partners.

Progress and Milestones

- Biocatalysis of phenolic polymers has been achieved on the bench-scale and could be available as a commercial process in the near term.
- The present effort will generate additional information needed to move enzymatic catalysis of polyphenols from the laboratory into scale-up.
- Data will be collected on the feasibility of enzymatic oxidation of alkenes to encourage industry to support a future demonstration project.
- Milestones for year one will include obtaining soluble and active hydrolase catalysts.
- A milestone of year two is to achieve a 100-fold activation for both enzymes in nonaqueous media.
- In year three, the majority of the research effort will be initiating process development for nonaqueous enzymatic catalysis.



PROJECT PARTNERS

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